=> d his

(FILE 'HOME' ENTERED AT 15:36:40 ON 08 JAN 2005)

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FILE 'REGISTRY' ENTERED AT 15:36:56 ON 08 JAN 2005
                STRUCTURE UPLOADED
Ll
L2
              1 S L1
L3
                STRUCTURE UPLOADED
              1 S L3
L4
                STRUCTURE UPLOADED
L5
L6
              2 S L5
L7
               STRUCTURE UPLOADED
              6 S L7
L8
           1268 S L7 SSS FULL
L9
     FILE 'CAPLUS' ENTERED AT 15:50:02 ON 08 JAN 2005
              2 S L9
L10
              0 S L10 NOT ISOQUINOLIN?
L11
                E BUNKER AMY/IN
L12
             11 S E3-E5
              1 S L12 AND AZAISOQUINOLIN?
L13
                STRUCTURE UPLOADED
L14
                S L14
     FILE 'REGISTRY' ENTERED AT 16:06:11 ON 08 JAN 2005
L15
              1 S L14
     FILE 'CAPLUS' ENTERED AT 16:06:12 ON 08 JAN 2005
L16
             1 S L15
     FILE 'REGISTRY' ENTERED AT 16:06:35 ON 08 JAN 2005
L17
              1 S L16 NOT L10
           1268 S L9 NOT L15
L18
             69 S L14 SSS FULL
L19
     FILE 'CAPLUS' ENTERED AT 16:08:37 ON 08 JAN 2005
L20
             2 S L19
    FILE 'BEILSTEIN' ENTERED AT 16:09:47 ON 08 JAN 2005
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L22 =>

L21

0 S L14

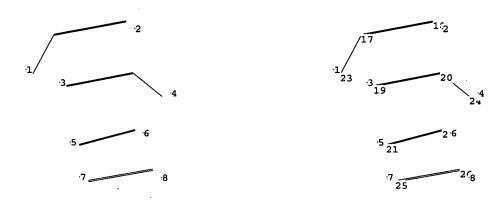
0 S L14 SSS FULL

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C:\STNEXP4\QUERIES\10634289c.str \(\angle 7\)
                                                                                              ak____1602
                                 a1____ a2
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```
chain nodes :
                                                               29 30 31 42 43 46 47
    13 14 15 16 17 18 19 20 21 22 23 24 26 27 28
ring nodes :
    1 2 3 4 5 6 7 8 9 10
chain bonds :
    3-42 7-47 8-46 13-14 15-16 16-17 18-19 20-21 21-22 23-24 26-27 28-29 30-31
    42-43
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
    1-2 1-6 2-3 3-4 3-42 4-5 5-6 6-10 7-47 8-9 8-46 9-10 13-14 15-16 16-17 18-19
    20-21 21-22 23-24 26-27 28-29 30-31 42-43
exact bonds :
    5-7 7-8
isolated ring systems :
    containing 1 :
G1:C,N
G2:C,O,S,N
G3: [*1-*2], [*3-*4], [*5-*6], [*7-*8], [*9-*10]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 13:CLASS
   14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 42:CLASS
```

43:Atom 46:CLASS 47:CLASS

Uploading C:\STNEXP4\QUERIES\1034289d.str L/4



```
chain nodes :
14  16  17  18  19  20  21  22  23  24  25  26  36
ring nodes :
1  2  3  4  5  6  7  8  9  10
chain bonds :
3-36  7-16  14-36  17-18  17-23  19-20  20-24  21-22  25-26
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10
exact/norm bonds :
1-2  1-6  2-3  3-4  3-36  4-5  5-6  6-10  7-16  8-9  9-10  14-36  17-18  17-23  19-20
20-24  21-22  25-26
exact bonds :
5-7  7-8
isolated ring systems :
containing 1 :
```

G1:C,N

G2:C,O,S,N

G3: [*1-*2], [*3-*4], [*5-*6], [*7-*8]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
14:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 36:CLASS

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=> d 1-2 bib abs hitstr
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ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
L20
     2004:143113 CAPLUS
AN
     140:175191
DN
     Azaisoquinoline derivatives as matrix metalloproteinase inhibitors,
TI
     pharmaceutical compositions, and therapeutic use
     Bunker, Amy Mae; Picard, Joseph Armand
IN
     Warner-Lambert Company LLC, USA
PΑ
     PCT Int. Appl., 132 pp.
so
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                               APPLICATION NO.
                                                                       DATE
                                  20040219
                                              WO 2003-IB3485
                                                                       20030804
ΡI
     WO 2004014866
                           A1
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT,
                          RO, RU, SC, SD, SE, SG, SK, SL,
                                                            TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE,
                          LS, MW, MZ, SD,
                                           SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
                 BJ, CF,
                          CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
                                  20040226
     US 2004038961
                           A1
                                              US 2003-634289
                                                                       20030805
PRAI US 2002-403219P
                           P
                                  20020813
     MARPAT 140:175191
AB
     The invention provides azaisoquinoline derivs., or pharmaceutically
     acceptable salts thereof. The invention also provides pharmaceutical
     compns. comprising a compound of the invention, or a pharmaceutically
     acceptable salt thereof, together with a pharmaceutically acceptable
     carrier, diluent, or excipient. The invention also provides methods of
     inhibiting an MMP-13 enzyme in an animal, comprising administering a
     compound of the invention, or a pharmaceutically acceptable salt thereof.
     The invention also provides methods of treating a disease mediated by an
     MMP-13 enzyme in a patient, comprising administering a compound of the
     invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition. The invention also provides methods for
     treating diseases such as heart disease, multiple sclerosis, osteo- and
     rheumatoid arthritis, arthritis other than osteo- or rheumatoid arthritis,
     cardiac insufficiency, inflammatory bowel disease, heart failure,
     age-related macular degeneration, chronic obstructive pulmonary disease,
     asthma, periodontal diseases, psoriasis, atherosclerosis, and osteoporosis
     in a patient, comprising administering to the patient a compound of the
     invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition The invention also provides combinations,
     comprising a compound of the invention, or a pharmaceutically acceptable
     salt thereof, together with another pharmaceutically active component.
     658036-97-6 658036-98-7 658036-99-8
     658037-00-4 658037-01-5 658037-02-6
     658037-03-7 658037-04-8
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (azaisoquinoline derivs. as matrix metalloproteinase inhibitors,
        pharmaceutical compns., and therapeutic use)
RN
     658036-97-6 CAPLUS
     1,6-Naphthyridin-5(6H)-one, 3-(3-phenyl-1-propynyl)-6-[[4-
CN
     (trifluoromethyl)phenyl]methyl] - (9CI) (CA INDEX NAME)
```

RN 658036-98-7 CAPLUS CN 1,6-Naphthyridin-5(6H)-one, 6-[(3-fluorophenyl)methyl]-3-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

RN 658036-99-8 CAPLUS

CN Benzoic acid, 4-[[3-[3-(1H-imidazol-1-yl)-1-propynyl]-5-oxo-1,6naphthyridin-6(5H)-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX

$$t-BuO-C$$
 CH_2-N
 $C=C-CH_2-N$
 N

658037-00-4 CAPLUS RN

Benzoic acid, 4-[[3-[3-(1H-imidazol-1-yl)-1-propynyl]-5-oxo-1,6-naphthyridin-6(5H)-yl]methyl]- (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2 CH_2

658037-01-5 CAPLUS

CN Benzonitrile, 3-[[1-oxo-7-(3-phenyl-1-propynyl)-2,6-naphthyridin-2(1H)yl]methyl] - (9CI) (CA INDEX NAME)

RN 658037-02-6 CAPLUS

CN Benzenesulfonamide, 4-[[1-oxo-7-(3-phenyl-1-propynyl)-2,6-naphthyridin-2(1H)-yl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \parallel \\ S-NH_2 \\ 0 \end{array}$$

RN

658037-03-7 CAPLUS
Benzoic acid, 4-[[1-oxo-7-[3-(1H-1,2,3-triazol-1-yl)-1-propynyl]-2,6-CN naphthyridin-2(1H)-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2 CH_2

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:142962 CAPLUS

DN 140:181338

TI Preparation of isoquinoline derivatives as matrix metalloproteinase inhibitors

IN Bunker, Amy Mae; Ortwine, Daniel Fred

PA Warner-Lambert Company Llc, USA

SO PCT Int. Appl., 189 pp.

CODEN: PIXXD2

DT Patent

LA English FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE PΙ WO 2004014379 A1 20040219 WO 2003-IB3521 20030804 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, PH, PL, PT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW LS, RW: GH, GM, KE, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2004044000 A1 20040304 US 2003-634473 20030805 PRAI US 2002-403031P 20020813

OS MARPAT 140:181338

GI

This invention provides compds. defined by formula (I) or pharmaceutically acceptable salts thereof [R1 = each (un)substituted C5 or C6 cycloalkyl-C1-6 alkylenyl, C8-10 bicycloalkyl-C1-8 alkylenyl, 5- or 6-membered heterocycloalkyl-C1-5 alkylenyl, 8- to 10-membered heterobicycloalkyl-C1-5 alkylenyl, phenyl-C1-8 alkylenyl, naphthyl-C1-8 alkylenyl, naphthyl-C1-8 alkylenyl, 5- or 6-membered heteroaryl-C1-8 alkylenyl, 8- to 10-membered heterobiaryl-C1-8 alkylenyl, Ph, naphthyl, etc.; R2 = H, C1-6 alkyl, each (un)substituted phenyl-C1-8 alkylenyl, naphthyl-C1-8 alkylenyl, 5- or 6-membered heteroaryl-C1-8 alkylenyl, or 8-

to 10-membered heterobiaryl-C1-8 alkylenyl, etc.; R3, R4 = H, each (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-6 cycloalkyl, C3-6 cycloalkyl-C1-8 alkylenyl, Ph, phenyl-C1-8 alkylenyl, naphthyl, naphthyl-C1-8 alkylenyl, 3- to 6-membered heterocycloalkyl, or 3- to 6-membered heterocycloalkyl-C1-8 alkylenyl, HO; C1-6 alkoxy, NH2, mono- or di(C1-6 alkyl)amino; R5 = H, C1-6 alkyl, NH2, HO, halo; n = an integer of 0-3; Q = OC(0), CH(R6)C(0), OC(NR6), CH(R6)C(NR6), N(R6)C(0), N(R6)C(S), N(R6)C(NR6), N(R6)CH2, SC(O), CH(R6)C(S), SC(NR6), trans- or cis-HC:CH, C.tplbond.C, CH2C.tplbond.C, C.tplbond.CCH2, etc.; R6 = H, C1-6 alkyl, C3-6 cycloalkyl, Ph, benzyl, etc.; Y = CO, CH2,CH(R7), C(R7)2, O, S, S(O), S(O)2; R7 = C1-6 alkyl, NH2, HO, halo]. The invention also provides pharmaceutical compns. comprising the compound I and the use of the compds. I for the manufacture of a medicament useful for treating osteoarthritis or rheumatoid arthritis. Thus, 4-(7-bromo-1-oxo-1H-isoquinolin-2ylmethyl)benzoic acid tert-Bu ester was coupled with 3-phenyl-1-propyne in the presence of CuI and Pd(Ph3P)4 in DMF at 65° for 5 h, followed by treatment with CF3CO2H to give 4-[1-oxo-7-(3-phenylprop-1-ynyl)-1Hisoquinolin-2-ylmethyl]benzoic acid (II). II showed IC50 of 0.0018 µM against MMP-13 catalytic domain. 658081-94-8P, 4-[(1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]methyl]benzoic acid tert-butyl ester RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; preparation of isoquinoline derivs. as matrix metalloproteinase inhibitors for treating osteoarthritis or rheumatoid arthritis)

RN

658081-94-8 CAPLUS Benzoic acid, 4-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ C-OBu-t \\ O \\ \end{array}$$

TT 658082-21-4P, 4-[[7-[3-(Imidazol-1-yl)prop-1-ynyl]-1-oxo-1Hisoquinolin-2-yl]methyl]benzoic acid tert-butyl ester 658082-25-8P , 4-[[1-0xo-7-[3-([1,2,4]triazol-1-yl)prop-1-ynyl]-1H-isoquinolin-2yl]methyl]benzoic acid tert-butyl ester 658082-27-0P, 4-[[4-Methyl-1-oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]methyl]benzoic acid tert-butyl ester RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of isoquinoline derivs. as matrix metalloproteinase inhibitors for treating osteoarthritis or rheumatoid arthritis) 658082-21-4 CAPLUS Benzoic acid, 4-[[7-[3-(1H-imidazol-1-yl)-1-propynyl]-1-oxo-2(1H)-RN CN

isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$t-BuO-C$$
 CH_2-N
 $C=C-CH_2-N$
 N

RN 658082-25-8 CAPLUS Benzoic acid, 4-[[1-oxo-7-[3-(1H-1,2,4-triazol-1-yl)-1-propynyl]-2(1H)-CN isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 658082-27-0 CAPLUS
CN Benzoic acid, 4-[[4-methyl-1-oxo-7-(3-phenyl-1-propynyl)-2(1H)isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{C-OBu-t} \\ \text{O} \\ \text{O} \end{array}$$

IT 658081-96-0P, 4-[[1-Oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]methyl]benzoic acid 658081-97-1P, 7-(3-Phenylprop-1-ynyl)-2-(4-trifluoromethylbenzyl)-2H-isoquinolin-1-one 658081-99-3P, 2-(3-Fluorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658082-01-0P, 3-[[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]methyl]benzonitrile 658082-03-2P, 4-[[1-0x0-7-(3-phenylprop-1ynyl)-1H-isoquinolin-2-yl]methyl]benzenesulfonamide 658082-05-4P , 4-[[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]methyl]benzoic acid methyl ester 658082-07-6P, 3-[[1-0xo-7-(3-phenylprop-1ynyl)-1H-isoquinolin-2-yl]methyl]benzoic acid methyl ester 658082-09-8P, 2-(4-Fluorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658082-11-2P, 7-(3-Phenylprop-1-ynyl)-2-(3trifluoromethylbenzyl)-2H-isoquinolin-1-one 658082-13-4P, 2-(3-Chlorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658082-15-6P, 2-(3,4-Difluorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658082-17-8P, 2-(3,5-Difluoro-4-hydroxybenzyl)-7-[3-(4H-[1,2,3]triazol-4-yl)prop-1-ynyl]-2H-isoquinolin-1-one 658082-23-6P, 4-[[7-[3-(Imidazol-1-yl)prop-1-ynyl]-1-oxo-1Hisoquinolin-2-yl]methyl]benzoic acid trifluoroacetate 658082-24-7P 4-[[1-0xo-7-(3-([1,2,3]triazol-1-yl)prop-1-ynyl)-1H-isoquinolin-2yl]methyl]benzoic acid tert-butyl ester 658082-26-9P, 4-[(1-0xo-7-[3-([1,2,4]triazol-1-yl)prop-1-ynyl]-1H-isoquinolin-2yl]methyl]benzoic acid 658082-31-6P, 4-[[4-Methyl-1-oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]methyl]benzoic acid 658082-32-7P, 7-(3-Phenylprop-1-ynyl)-2-[4-(2H-tetrazol-5yl)benzyl]-2H-isoquinolin-1-one 658082-35-0P, 4-[[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]methyl]-N-(piperidin-1-yl) benzamide 658082-36-1P, N-[2-(Morpholin-4-yl)ethyl]-4-[[1-oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]methyl] benzamide 658082-37-2P, N-(5-0xo-4,5-dihydro-1H-pyrazol-3-yl)-4-[[1-oxo-7-(3phenylprop-1-ynyl)-1H-isoquinolin-2-yl]methyl]benzamide 658083-00-2P, 7-(3-Phenylprop-1-ynyl)-2-[(tetrahydropyran-2yl)methyl]-2H-isoquinolin-1-one 658083-01-3P, 2-[3-Hydroxy-2,2-bis(hydroxymethyl)propyl]-7-(3-phenylprop-1-ynyl)-2Hisoquinolin-1-one 658083-02-4P, 3-[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]propionitrile 658083-03-5P 2-(2,3-Dihydroxypropyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-04-6P, 2-[2-(1,3-Dioxinan-2-yl)ethyl]-7-(3-phenylprop-1ynyl)-2H-isoquinolin-1-one 658083-05-7P, 4-[1-0x0-7-(3phenylprop-1-ynyl)-1H-isoquinolin-2-yl]butyronitrile 658083-06-8P 2-(2-Methyltetrahydropyran-3-yl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-07-9P, 2-(2,2-Dimethoxyethyl)-7-(3-phenylprop-1ynyl)-2H-isoquinolin-1-one 658083-08-0P, 7-(3-Phenylprop-1-ynyl)-2-[(tetrahydrofuran-2-yl)methyl]-2H-isoquinolin-1-one 658083-09-1P 5-[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]pentanenitrile 658083-10-4P, 3-[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]propionic acid methyl ester 658083-11-5P, Acetic acid 4-[1-oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]butyl ester 658083-12-6P, 2-[2-(1,3-Dioxolan-2-yl)ethyl]-7-(3-phenylprop-1ynyl)-2H-isoquinolin-1-one 658083-13-7P, 2-(1,3-Dioxolan-2yl)methyl-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one

RN

CN

658083-14-8P, 2-[4-(Methanesulfonyl)benzyl]-7-(3-phenylprop-1ynyl)-2H-isoquinolin-1-one 658083-15-9P, 5-[1-Oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]pentanoic acid methyl ester 658083-16-0P, [1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]acetic acid methyl ester 658083-17-1P, 2-(2,2-Diethoxyethyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-18-2P, 5-[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]pentanoic acid ethyl ester 658083-19-3P, 3-[1-0x0-7-(3-phenylprop-1-ynyl)-1Hisoquinolin-2-yl]propionic acid ethyl ester 658083-20-6P, 7-Methoxy-3-[[1-oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2-yl]methyl]-1,4-benzoxazin-2-one 658083-21-7P, 6-[1-0xo-7-(3-phenylprop-1ynyl)-1H-isoquinolin-2-yl]hexanoic acid ethyl ester 658083-22-8P , 2-(2-Methoxyethyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-23-9P, [1-Oxo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]acetic acid ethyl ester 658083-24-0P, 2-(3-Hydroxy-2,2dimethylpropyl) -7-(3-phenylprop-1-ynyl) -2H-isoquinolin-1-one 658083-25-1P, 2-[2-(Benzenesulfinyl)ethyl]-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-26-2P, 4-[1-0xo-7-(3-phenylprop-1ynyl)-1H-isoquinolin-2-yl]butyric acid ethyl ester 658083-27-3P, 2-(2-Oxobutyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-28-4P, 2-(6-Hydroxyhexyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-29-5P, 2-Benzenesulfonylmethyl-7-(3phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-30-8P, 2-(3,3-Dimethyl-2-oxobutyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-31-9P, 6-[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]hexanenitrile 658083-32-0P, 2-Benzyl-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-1-one 658083-33-1P, 7-(3-Phenylprop-1-ynyl)-2-(2,2,2-trifluoroethyl)-2H-isoquinolin-1-one 658083-34-2P, 7-(3-Phenylprop-1-ynyl)-2-(4,4,4-trifluorobutyl)-2H-isoquinolin-1-one 658083-35-3P, 7-[1-0xo-7-(3-phenylprop-1-ynyl)-1H-isoquinolin-2yl]heptanenitrile RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of isoquinoline derivs. as matrix metalloproteinase inhibitors for treating osteoarthritis or rheumatoid arthritis) 658081-96-0 CAPLUS Benzoic acid, 4-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)isoquinolinyl]methyl] - (9CI) (CA INDEX NAME)

$$Ph-CH_2-C$$
 CH_2 CH_2 CH_2

RN 658081-97-1 CAPLUS
CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 658081-99-3 CAPLUS CN 1(2H)-Isoquinolinone, 2-[(3-fluorophenyl)methyl]-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

$$Ph-CH_2-C$$

658082-01-0 CAPLUS
Benzonitrile, 3-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME) CN

658082-03-2 CAPLUS RN

CN Benzenesulfonamide, 4-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)isoquinolinyl]methyl] - (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$

$$N-CH_2$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

$$0$$

RN

658082-05-4 CAPLUS Benzoic acid, 4-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-CN isoquinolinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ C \\ C \\ O \end{array}$$

RN

658082-07-6 CAPLUS Benzoic acid, 3-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-CN isoquinolinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 658082-09-8 CAPLUS

CN 1(2H)-Isoquinolinone, 2-[(4-fluorophenyl)methyl]-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

658082-11-2 CAPLUS

1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME) CN

658082-13-4 CAPLUS RN

1(2H)-Isoquinolinone, 2-[(3-chlorophenyl)methyl]-7-(3-phenyl-1-propynyl)-CN (9CI) (CA INDEX NAME)

RN 658082-15-6 CAPLUS

1(2H)-Isoquinolinone, 2-[(3,4-difluorophenyl)methyl]-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C$$
 C N CH_2 N

RN 658082-17-8 CAPLUS

CN 1(2H)-Isoquinolinone, 2-[(3,5-difluoro-4-hydroxyphenyl)methyl]-7-[3-(4H-1,2,3-triazol-4-yl)-1-propynyl]- (9CI) (CA INDEX NAME)

658082-23-6 CAPLUS
Benzoic acid, 4-[[7-[3-(1H-imidazol-1-yl)-1-propynyl]-1-oxo-2(1H)-isoquinolinyl]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM

RN

CRN 658082-22-5 CMF C23 H17 N3 O3

$$CH_2$$
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2

CRN 76-05-1 CMF C2 H F3 O2

RN

658082-24-7 CAPLUS Benzoic acid, 4-[[1-oxo-7-[3-(1H-1,2,3-triazol-1-yl)-1-propynyl]-2(1H)-CN isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$c = c - cH_2 - N$$

RN

658082-26-9 CAPLUS Benzoic acid, 4-[[1-oxo-7-[3-(1H-1,2,4-triazol-1-yl)-1-propynyl]-2(1H)-CN isoquinolinyl]methyl] - (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2 CH_2

RN 658082-31-6 CAPLUS

CN Benzoic acid, 4-[[4-methyl-1-oxo-7-(3-phenyl-1-propynyl)-2(1H)isoquinolinyl]methyl] - (9CI) (CA INDEX NAME)

RN 658082-32-7 CAPLUS

1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[[4-(1H-tetrazol-5-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 658082-35-0 CAPLUS

Benzamide, 4-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-isoquinolinyl]methyl]-N-1-piperidinyl- (9CI) (CA INDEX NAME) CN

RN 658082-36-1 CAPLUS

CN Benzamide, N-[2-(4-morpholinyl)ethyl]-4-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \text{C-NH-CH}_2\text{-CH}_2 \end{array}$$

658082-37-2 CAPLUS

RN

CN Benzamide, N-(4,5-dihydro-5-oxo-1H-pyrazol-3-yl)-4-[{1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)

$$\mathsf{Ph}-\mathsf{CH}_2-\mathsf{C}=\mathsf{C}$$

RN 658083-00-2 CAPLUS

CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[(tetrahydro-2H-pyran-2yl)methyl]- (9CI) (CA INDEX NAME)

RN 658083-01-3 CAPLUS

CN 1(2H)-Isoquinolinone, 2-[3-hydroxy-2,2-bis(hydroxymethyl)propyl]-7-(3phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$
 CH_2-OH
 CH_2-CH_2-OH
 CH_2-OH

RN 658083-02-4 CAPLUS

CN 2(1H)-Isoquinolinepropanenitrile, 1-oxo-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

RN 658083-03-5 CAPLUS CN 1(2H)-Isoquinolinone, 2-(2,3-dihydroxypropyl)-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

RN 658083-04-6 CAPLUS CN 1(2H)-Isoquinolinone, 2-[2-(1,3-dioxan-2-yl)ethyl]-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

$$Ph-CH_2-C=C$$

RN 658083-05-7 CAPLUS CN 2(1H)-Isoquinolinebutanenitrile, 1-oxo-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C=C$$
 C
 N
 $(CH_2)_3-CN$

RN 658083-06-8 CAPLUS
CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-(tetrahydro-2-methyl-2H-pyran-3-yl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C \equiv C$$

RN 658083-07-9 CAPLUS CN 1(2H)-Isoquinolinone, 2-(2,2-dimethoxyethyl)-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

$$_{\mathrm{Ph-CH_{2}-C}}$$

RN 658083-08-0 CAPLUS

CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[(tetrahydro-2furanyl)methyl]- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$
 $N-CH_2$

RN 658083-09-1 CAPLUS

CN 2(1H)-Isoquinolinepentanenitrile, 1-oxo-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

RN 658083-10-4 CAPLUS

RN 658083-11-5 CAPLUS

CN 1(2H)-Isoquinolinone, 2-[4-(acetyloxy)butyl]-7-(3-phenyl-1-propynyl)(9CI) (CA INDEX NAME)

RN 658083-12-6 CAPLUS

CN 1(2H)-Isoquinolinone, 2-[2-(1,3-dioxolan-2-yl)ethyl]-7-(3-phenyl-1propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C \qquad N - CH_2-CH_2 - O$$

RN 658083-13-7 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(1,3-dioxolan-2-ylmethyl)-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

658083-14-8 CAPLUS RN

1(2H)-Isoquinolinone, 2-[[4-(methylsulfonyl)phenyl]methyl]-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ S-Me \\ 0 \end{array}$$

658083-15-9 CAPLUS

RN2(1H)-Isoquinolinepentanoic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, methyl CN ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$
 $(CH_2)_4-C-OMe$

RN 658083-16-0 CAPLUS

2(1H)-Isoquinolineacetic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, methyl CN ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$
 $CH_2-C-OMe$

RN 658083-17-1 CAPLUS

1(2H)-Isoquinolinone, 2-(2,2-diethoxyethyl)-7-(3-phenyl-1-propynyl)- (9CI) CN (CA INDEX NAME)

RN 658083-18-2 CAPLUS

2(1H)-Isoquinolinepentanoic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 658083-19-3 CAPLUS

CN 2(1H)-Isoquinolinepropanoic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 658083-20-6 CAPLUS

CN 2H-1,4-Benzoxazin-2-one, 7-methoxy-3-[[1-oxo-7-(3-phenyl-1-propynyl)-2(1H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)

$$\mathsf{Ph}\mathsf{-}\mathsf{CH}_2\mathsf{-}\mathsf{C} = \mathsf{C} \\ \\ \mathsf{O} \\ \\ \mathsf{N}\mathsf{-}\mathsf{CH}_2 \\ \\ \mathsf{N} \\ \\ \mathsf{N} \\ \\ \mathsf{OMe}$$

RN 658083-21-7 CAPLUS

CN 2(1H)-Isoquinolinehexanoic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, ethyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C \qquad \qquad C \qquad$$

RN 658083-22-8 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(2-methoxyethyl)-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$\mathsf{Ph}\mathsf{-}\mathsf{CH}_2\mathsf{-}\mathsf{C} = \mathsf{C} \\ \mathsf{C} \\ \mathsf{N} \\ \mathsf{CH}_2\mathsf{-}\mathsf{CH}_2\mathsf{-}\mathsf{OMe}$$

RN 658083-23-9 CAPLUS

CN 2(1H)-Isoquinolineacetic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 658083-24-0 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(3-hydroxy-2,2-dimethylpropyl)-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

RN 658083-25-1 CAPLUS CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[2-(phenylsulfinyl)ethyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
0 & \\
Ph-S-CH_2-CH_2
\end{array}$$

$$\begin{array}{c}
C = C-CH_2-Ph
\end{array}$$

RN 658083-26-2 CAPLUS

CN 2(1H)-Isoquinolinebutanoic acid, 1-oxo-7-(3-phenyl-1-propynyl)-, ethyl ester (9CI) (CA INDEX NAME)

Ph-CH₂-C=C
$$(CH_2)_3$$
-C-OEt

RN 658083-27-3 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(2-oxobutyl)-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$

$$CH_2-C-Et$$

RN 658083-28-4 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(6-hydroxyhexyl)-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

RN 658083-29-5 CAPLUS

CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[(phenylsulfonyl)methyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ Ph-S-CH_2 & \\ O & \\ \end{array}$$

RN 658083-30-8 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(3,3-dimethyl-2-oxobutyl)-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

$$Ph-CH_2-C=C$$

$$CH_2-C-Bu-t$$

RN 658083-31-9 CAPLUS

CN 2(1H)-Isoquinolinehexanenitrile, 1-oxo-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C=C$$
 $CH_2)_5-CN$

RN 658083-32-0 CAPLUS

CN 1(2H)-Isoquinolinone, 2-(phenylmethyl)-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2$$
 $C = C-CH_2-Ph$

RN 658083-33-1 CAPLUS

CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-(2,2,2-trifluoroethyl)(9CI) (CA INDEX NAME)

$$Ph-CH_2-C=C$$
 CH_2-CF_3

RN 658083-34-2 CAPLUS

CN 1(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-(4,4,4-trifluorobutyl)(9CI) (CA INDEX NAME)

$$Ph-CH_2-C = C$$

(CH₂)₃-CF₃

RN 658083-35-3 CAPLUS

$$Ph-CH_2-C = C$$
 $(CH_2)_6-CN$

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

GI

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ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
     2002:615576 CAPLUS
AN
     137:169431
DN
ΤI
     Preparation of isoquinolinones as dipeptidyl peptidase IV inhibitors for
     the prophylaxis or treatment of diabetes
     Oi, Satoru; Ikedou, Koji; Takeuchi, Koji; Ogino, Masaki; Banno, Yoshihiro; Tawada, Hiroyuki; Yamane, Taihei
IN
PA
     Takeda Chemical Industries, Ltd., Japan
SO
     PCT Int. Appl., 600 pp.
     CODEN: PIXXD2
ידים
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                              APPLICATION NO.
                                                                       DATE
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ΡI
     WO 2002062764
                           A1
                                  20020815
                                              WO 2002-JP831
                                                                       20020201
                                  20021010
     WO 2002062764
                           C2
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             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
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                          SD, SE, SG, SI,
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             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
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     CA 2437492
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                                                                       20020201
     JP 2003238566
                           A2
                                  20030827
                                              JP 2002-26185
                                                                       20020201
                                  20031029
                                              EP 2002-711278
     EP 1355886
                           A1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002006831
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                                  20030930
                                              NO 2003-3385
                                                                       20030729
     US 2004082607
                           A1
                                  20040429
                                              US 2003-470805
                                                                       20030801
PRAI JP 2001-27349
                                  20010202
                           Α
     JP 2001-292388
                           Α
                                  20010925
     JP 2001-382232
                                  20011214
     WO 2002-JP831
                                  20020201
     MARPAT 137:169431
os
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III

AB Title compds. I [R1, R2 = (un) substituted alkyl or heterocyclic ring; A = (un) substituted 5 to 10-membered aromatic ring; X = bond, O, S, etc.; L = divalent hydrocarbon or a salt], their pharmaceutically acceptable salts and formulations were prepared For example, acylation of amino isoquinolinone II, followed by BOC deprotection provided claimed isoquinolinone III.HCl. Isoquinolinone III inhibited human dipeptidyl peptidase V with an IC50 = 0.25 μM. Also, the plasma glucose-lowering (76%) and insulinotropic effects (255%) of III in rat were reported. Compds. I have superior peptidase inhibitory activity and are useful for the prophylaxis or treatment of diabetes.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d l10 2 bib abs hitstr
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L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
     2001:152935 CAPLUS
DN
     134:193349
ΤI
     Preparation and antimicrobial activities of combinatorial libraries of
     4-unsubstituted dihydroisoquinolinone derivatives
IN
     Motesharei, Kianoush; Lebl, Michal; Krchnak, Viktor; Ni, Yidong
PΑ
     Trega Biosciences, Inc., USA
     PCT Int. Appl., 162 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                             APPLICATION NO.
                                                                    DATE
ΡI
     WO 2001014879
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                                             WO 2000-US20774
                          A1
                                                                    20000728
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
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     US 6452009
                                 20020917
                                             US 1999-378569
                          B1
     EP 1210598
                          A1
                                20020605
                                             EP 2000-955287
                                                                    20000728
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             IE, FI, CY
PRAI US 1999-378569
                                19990819
     WO 2000-US20774
                                20000728
os
     MARPAT 134:193349
GT
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$$\begin{array}{c|c}
X & Y \\
R^{1} (CO)_{n} N & R^{3} \\
& Z & O
\end{array}$$

$$\begin{array}{c}
R^{4} (CO)_{p} R^{5} R^{6} R^{7} \\
& CO)_{m} R^{2}
\end{array}$$

dihydroisoquinolinones)

RN

Dihydroisoquinolinones I [R1, R2 = H, alkyl, alkenyl, Ph, etc.; R3 = H, alkyl, heteroaryl, etc.; R4 = -, DWE and W = -, cycloalkyene, arylene, etc. and D and E = -, alkylene, alkynylene, etc.; R5 = -, O, S, amino; R6 - -, alkylene, alkenylene; R7 = H, halide, OR13, CO2R13, etc.; X, Y, Z = H, halo, OH, cyano, nitro, etc.; m, n, p = 0, 1 and when 0 the absent carbonyl can be replaced with SO2] were prepared Thus, bromoacetic acid was coupled to a resin and the resulting compds. were coupled with 1,4-Boc-NH-CH2-Ph-COOH, deprotected, and reacted with an aldehyde. resulting compds. were then reacted with 4-nitrohomophthalic acid, reduced with tin chloride, and the compds. were reacted with a carboxylic acid. The resulting compds. were then cleaved and extracted The melanocortin receptor assay and antimicrobial activity of I were investigated. 316794-00-0P 316794-18-0P 316794-26-0P 317837-21-1P 317860-47-2P 318282-92-7P 328058-84-0P 328058-89-5P 328058-90-8P 328058-92-0P 328059-00-3P 328059-01-4P 328059-17-2P 328059-20-7P 328059-26-3P 328059-27-4P 328059-28-5P 328059-31-0P 328059-35-4P 328059-40-1P 328059-50-3P 328059-51-4P 328059-59-2P 328059-60-5P 328059-63-8P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antimicrobial activities of combinatorial libraries of

Ι

316794-00-0 CAPLUS
2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-1-oxo-3-phenyl-7-[[(1-phenylcyclopropyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 316794-18-0 CAPLUS
CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-7-[(4-iodobenzoyl)amino]-1-oxo-3-(2-quinolinyl)- (9CI) (CA INDEX NAME)

RN 316794-26-0 CAPLUS
CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-7-[(4-iodobenzoyl)amino]-1-oxo-3-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 317837-21-1 CAPLUS
CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-7-[(2-furanylcarbonyl)amino]-3,4-dihydro-3-(1-naphthalenyl)-1-oxo-(9CI) (CA INDEX NAME)

RN 317860-47-2 CAPLUS
CN Benzamide, N-(2-amino-2-oxoethyl)-4-[[7-[(2,6-difluorobenzoyl)amino]-3-[4-(1,1-dimethylethyl)phenyl]-3,4-dihydro-1-oxo-2(1H)-isoquinolinyl]methyl]-N-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

RN 318282-92-7 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-7-[[2-fluoro-3-(trifluoromethyl)benzoyl]amino]-3,4-dihydro-1-oxo-3-phenyl- (9CI) (CA INDEX NAME)

RN 328058-84-0 CAPLUS

N 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2 (dimethylamino)ethyl]-7-[[2-fluoro-3-(trifluoromethyl)benzoyl]amino]-3,4 dihydro-1-oxo-3-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 328058-89-5 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3,5-dimethoxyphenyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-7-[[(4-methylcyclohexyl)carbonyl]amino]-1-oxo-(9CI) (CA INDEX NAME)

RN 328058-90-8 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3-[4-[3-(dimethylamino)propoxy]phenyl]-3,4-dihydro-7-[(4-iodobenzoyl)amino]-1-oxo-(9CI) (CA INDEX NAME)

RN 328058-92-0 CAPLUS
CN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-[4-[3-(dimethylamino)propoxy]phenyl]-3,4-dihydro-1-oxo-7-[[4-(trifluoromethoxy)benzoyl]amino]-2(1H)-isoquinolinyl]methyl]-N-propyl-(9CI) (CA INDEX NAME)

RN 328059-00-3 CAPLUS
CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3,5-dimethoxyphenyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-1-oxo-7-[[4-(trifluoromethoxy)benzoyl]amino]- (9CI) (CA INDEX NAME)

RN 328059-01-4 CAPLUS
CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(3,4-difluorobenzoyl)amino]-3-(3,5-dimethoxyphenyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-1-oxo- (9CI) (CA INDEX NAME)

RN 328059-17-2 CAPLUS
CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[[3,5-bis(trifluoromethyl)benzoyl]amino]-3-(3,4-difluorophenyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-20-7 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[[3,5-bis(trifluoromethyl)benzoyl]amino]-N-[2-(dimethylamino)ethyl]-3,4-dihydro-3-(4-methylphenyl)-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-26-3 CAPLUS

2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-3-(1-naphthalenyl)-1-oxo-7-[(pyrazinylcarbonyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ \hline \\ N & & \\ N & & \\ \end{array} \begin{array}{c} O & CH_2-CH_2-NMe_2 \\ \hline \\ CH_2-CH_2-C-N-CH_2-C-NH_2 \\ \hline \\ O & \\ \end{array}$$

RN 328059-27-4 CAPLUS

CN

2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-3-(1-naphthalenyl)-1-oxo-7-[[(1-phenylcyclopropyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

$$\bigcap_{Ph}^{O} \bigcap_{C-NH}^{O} \bigcap_{N}^{CH_2-CH_2-NMe_2} \bigcap_{CH_2-CH_2-C-NH_2}^{O} \bigcap_{N}^{CH_2-CH_2-C-NH_2} \bigcap_{N}^{O} \bigcap_{N}^{CH_2-CH_2-C-NH_2}$$

328059-28-5 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-7-[[(4-methyl-1,2,3-thiadiazol-5-yl)carbonyl]amino]-3-(1-naphthalenyl)-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-31-0 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3-[4-[3-(dimethylamino)propoxy]phenyl]-3,4-dihydro-7-[[(4-methylcyclohexyl)carbonyl]amino]-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-35-4 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-[4-[3-(dimethylamino)propoxy]phenyl]-3,4-dihydro-7-[(4-iodobenzoyl)amino]-1-oxo-N-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

328059-40-1 CAPLUS

RN

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(3,4-difluorobenzoyl)amino]-N-[2-(dimethylamino)ethyl]-3-[4-(1,1-dimethylethyl)phenyl]-3,4-dihydro-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-50-3 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(4-cyanobenzoyl)amino]-N-[2-(dimethylamino)ethyl]-3-[4-(1,1-dimethylethyl)phenyl]-3,4-dihydro-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-51-4 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3-[4-(1,1-dimethylethyl)phenyl]-3,4-dihydro-7-[[(5-methylpyrazinyl)carbonyl]amino]-1-oxo-(9CI) (CA INDEX NAME)

N 328059-59-2 CAPLUS

N 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[[3,5-bis(trifluoromethyl)benzoyl]amino]-N-[2-(dimethylamino)ethyl]-3,4-dihydro-1-oxo-3-(2-quinolinyl)- (9CI) (CA INDEX NAME)

$$F_{3}C$$

$$CF_{3}$$

$$CH_{2}-CH_{2}-CH_{2}-NH_{2}$$

$$CH_{2}-CH_{2}-C-NH_{2}$$

$$CH_{2}-CH_{2}-C-NH_{2}$$

RN 328059-60-5 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2-(dimethylamino)ethyl]-3-[4-(1,1-dimethylethyl)phenyl]-7-[(2-fluorobenzoyl)amino]-3,4-dihydro-1-oxo-(9CI) (CA INDEX NAME)

RN 328059-63-8 CAPLUS

CN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3,5-dimethoxyphenyl)-N-[2-(dimethylamino)ethyl]-3,4-dihydro-1-oxo-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino]- (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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> s e3-e5
              1 "BUNKER AMY"/IN
              2 "BUNKER AMY M"/IN
              8 "BUNKER AMY MAE"/IN
             11 ("BUNKER AMY"/IN OR "BUNKER AMY M"/IN OR "BUNKER AMY MAE"/IN)
L12
=> s 112 and azaisoquinolin?
              1 AZAISOQUINOLIN?
              1 L12 AND AZAISOOUINOLIN?
L13
=> d bib abs
     ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
L13
     2004:143113 CAPLUS
AN
DN
     140:175191
     Azaisoquinoline derivatives as matrix metalloproteinase
     inhibitors, pharmaceutical compositions, and therapeutic use
IN
     Bunker, Amy Mae; Picard, Joseph Armand
PA
     Warner-Lambert Company LLC, USA
     PCT Int. Appl., 132 pp.
     CODEN: PIXXD2
דת
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                           KIND
                                  DATE
                                               APPLICATION NO.
                                                                        DATE
PΙ
     WO 2004014866
                           A1
                                  20040219
                                               WO 2003-IB3485
                                                                        20030804
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
              LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
              PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
              TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
              KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
              FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
              BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2004038961
                                  20040226
                           AΊ
                                               US 2003-634289
                                                                        20030805
PRAI US 2002-403219P
                            P
                                  20020813
     MARPAT 140:175191
     The invention provides azaisoquinoline derivs., or
     pharmaceutically acceptable salts thereof. The invention also provides
     pharmaceutical compns. comprising a compound of the invention, or a
     pharmaceutically acceptable salt thereof, together with a pharmaceutically
     acceptable carrier, diluent, or excipient. The invention also provides methods of inhibiting an MMP-13 enzyme in an animal, comprising
     administering a compound of the invention, or a pharmaceutically acceptable
     salt thereof. The invention also provides methods of treating a disease
     mediated by an MMP-13 enzyme in a patient, comprising administering a
     compound of the invention, or a pharmaceutically acceptable salt thereof,
     either alone or in a pharmaceutical composition. The invention also provides
     methods for treating diseases such as heart disease, multiple sclerosis,
     osteo- and rheumatoid arthritis, arthritis other than osteo- or rheumatoid
     arthritis, cardiac insufficiency, inflammatory bowel disease, heart
     failure, age-related macular degeneration, chronic obstructive pulmonary
     disease, asthma, periodontal diseases, psoriasis, atherosclerosis, and
     osteoporosis in a patient, comprising administering to the patient a
     compound of the invention, or a pharmaceutically acceptable salt thereof, either alone or in a pharmaceutical composition. The invention also provides
     combinations, comprising a compound of the invention, or a pharmaceutically
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RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

acceptable salt thereof, together with another pharmaceutically active

=> d re

component.

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L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
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⁽¹⁾ Eisai Co Ltd; EP 0722936 A 1996 CAPLUS (2) Hayashizaki, Y; WO 0244195 A 2002 CAPLUS

⁽³⁾ Univ Boston; WO 0196607 A 2001 CAPLUS